



chain nodes :  
 1 2 3 4 5 6 18 19 22  
 ring nodes :  
 9 10 11 12 13 14  
 chain bonds :  
 1-2 1-19 2-3 2-4 4-5 5-6 6-13 10-18  
 ring bonds :  
 9-10 9-14 10-11 11-12 12-13 13-14  
 exact/norm bonds :  
 2-3 2-4 5-6 6-13 10-18  
 exact bonds :  
 1-2 1-19 4-5  
 normalized bonds :  
 9-10 9-14 10-11 11-12 12-13 13-14

G1:CN,NO2,F,S,CO2H,CHO

G2:O,N

G3:C,Hy,Ak

Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 18:CLASS 19:CLASS 22:CLASS 23:CLASS